DIFFRACTION GRATING MONOCHROMATORS (PGMs)

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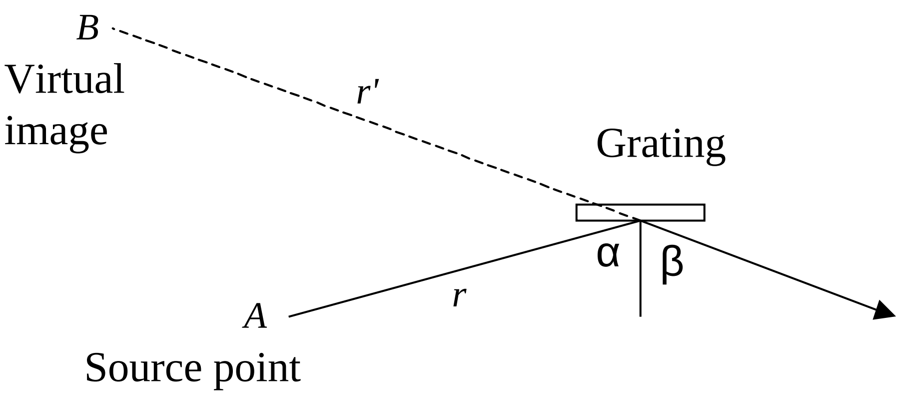
Advanced Light Source

PLANE GRATING SYSTEMS: GENERAL



Eliminating α between

$$\frac{m\lambda}{d_0} = \sin\alpha + \sin\beta \quad \text{and} \quad c_{ff} = \frac{\cos\beta}{\cos\alpha}$$

$$\sin\beta = \frac{\dfrac{m\lambda}{d} - \sqrt{\left(\dfrac{m\lambda}{d}\right)^2 \dfrac{1}{c_{ff}^2} + \left(1 - \dfrac{1}{c_{ff}^2}\right)^2}}{\left(1 - \dfrac{1}{c_{ff}^2}\right)}$$

Focus condition for a spherical grating

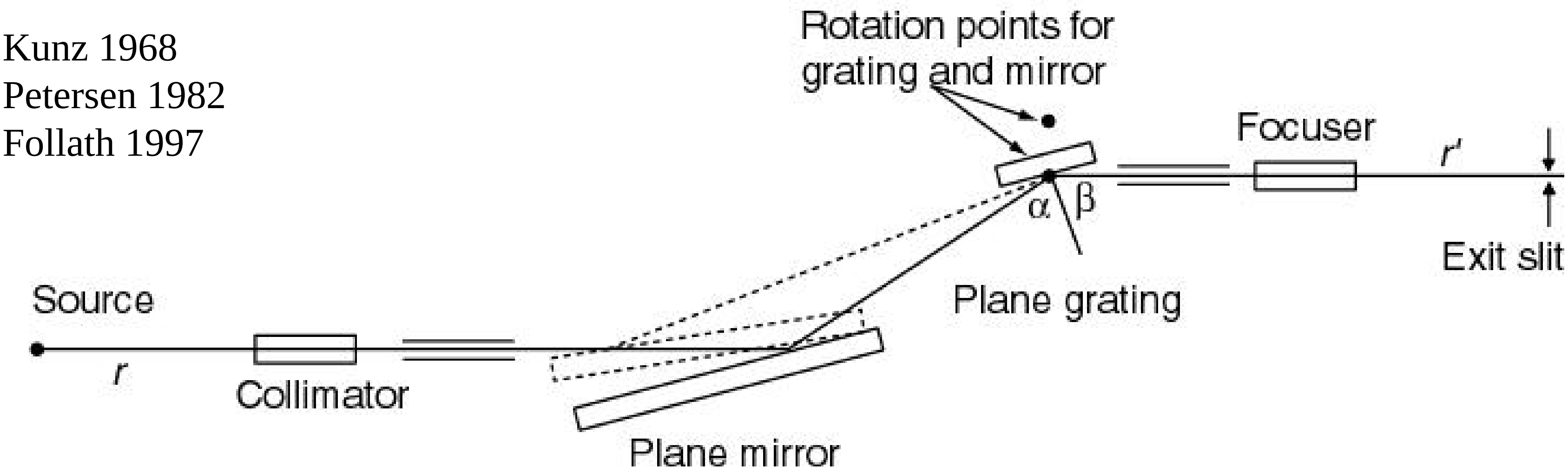
$$\left(\frac{\cos^2\alpha}{r} - \frac{\cos\alpha}{R}\right) + \left(\frac{\cos^2\beta}{r'} - \frac{\cos\beta}{R}\right) = 0 \qquad \text{let } R \rightarrow \infty \quad \rightarrow \quad r' = -r\frac{\cos^2\beta}{\cos^2\alpha}$$

Note that if $r = \infty$ then $r' = \infty$ irrespective of c_{ff} i.e . the grating then does no focusing

Using $c_{ff} = \dfrac{\cos\beta}{\cos\alpha}$ and recalling that $M = -\dfrac{r'}{r}\dfrac{\cos\alpha}{\cos\beta}$ $\rightarrow$ $\boxed{M = c_{ff}}$ (of the grating alone)

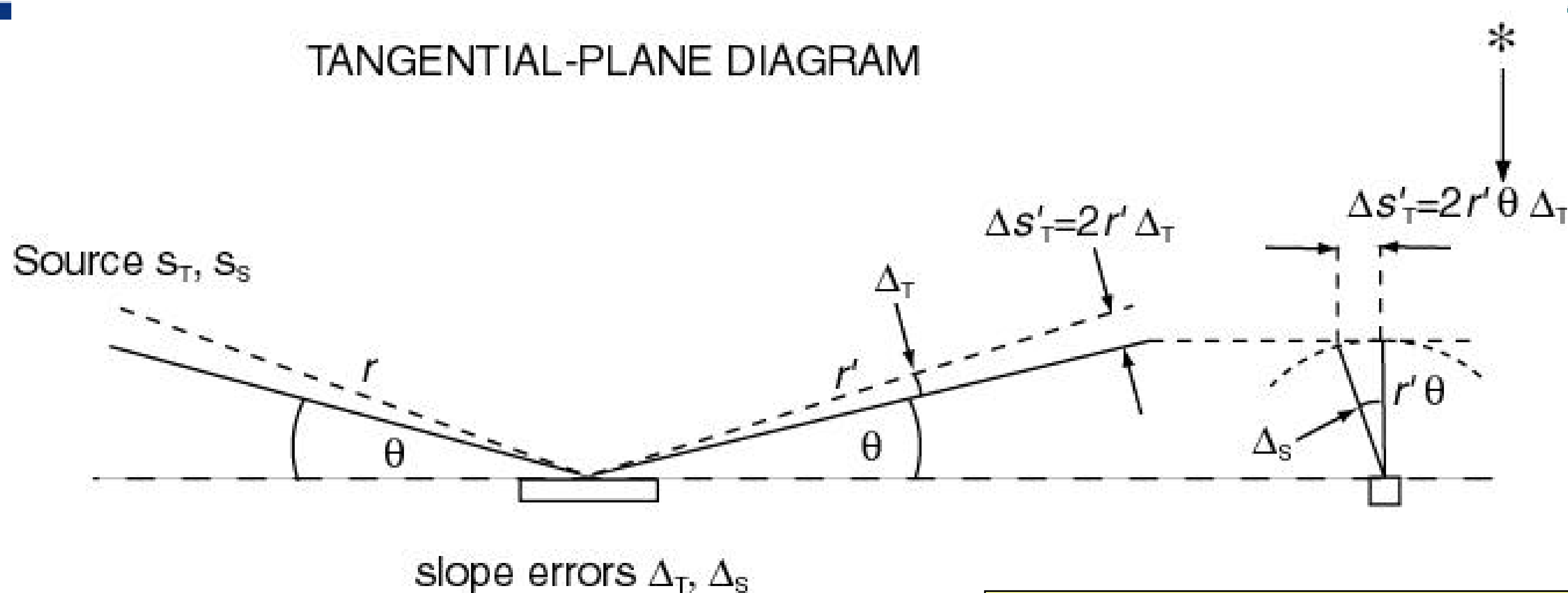
COLLIMATED LIGHT SX700 (CLSX700)

Kunz 1968
Petersen 1982
Follath 1997



- This is the current and deservedly the most popular of many versions (used in ALS MES project)
- The original (Petersen) held fixed focus by maintaining $c_{\mathrm{ff}} = \cos\beta / \cos\alpha = 2.25$ and introduced the still-essential mechanism for positioning the plane mirror (next slide)
- CLSX700 has constant focus position *irrespective* of the value of c_{ff} which therefore becomes a user-controlled variable
- This can be used to track the efficiency maximum, suppress high orders or maximize resolution
- Sagittal focusing mirrors reduce sensitivity to manufacturing errors (Jark 1992) see next slide, other types were paraboloid (Kunz 1968), ellipsoid (Petersen 1982), elliptical cylinder (Nyholm 1985) or sphere (Padmore 1989)

FORGIVENESS FACTOR



Requirement: $\Delta s'_T \le \frac{1}{2} s'_T \quad \rightarrow \quad 2r'\Delta_T \le \frac{1}{2}\frac{r'}{r} s_T$

$$\boxed{\Delta_T \le \frac{1}{4}\frac{s_T}{r}}$$

$$\Delta s'_S \le \frac{1}{2} s'_S \quad \rightarrow \quad 2r'\theta\Delta_S \le \frac{1}{2}\frac{r'}{r} s_S$$

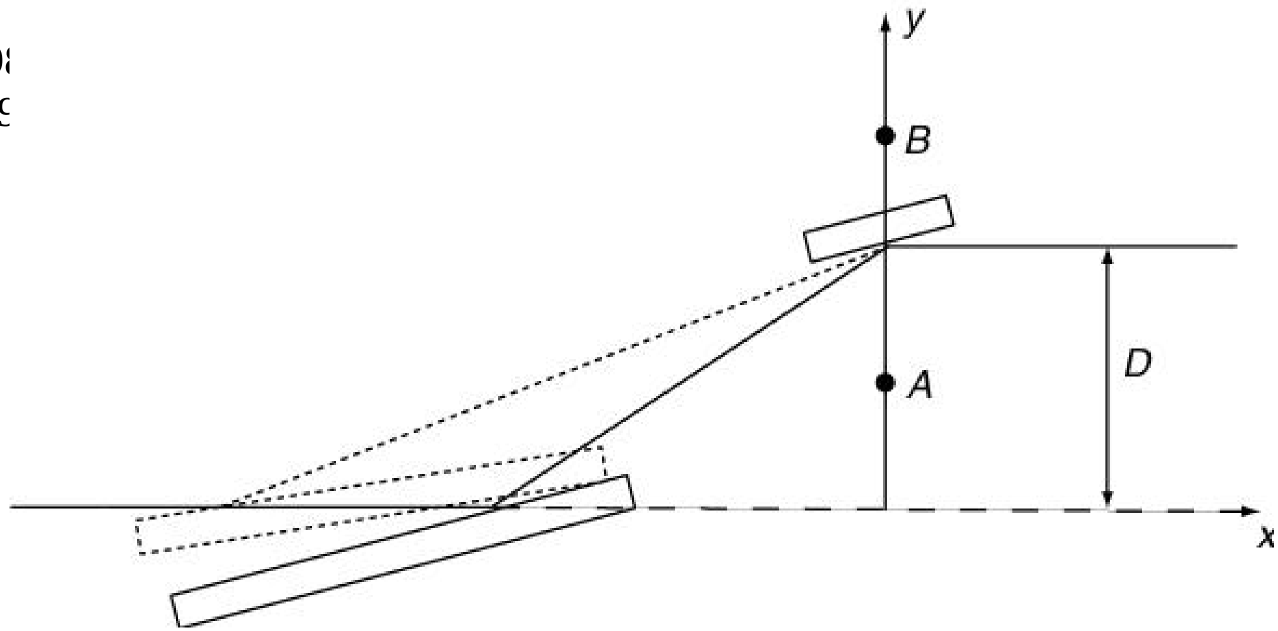
$$\boxed{\Delta_S \le \frac{1}{4}\frac{s_S}{r\theta}}$$

Reasons for the factor 2's:

1. Ray deviation is twice that of the mirror
2. Quadratic sum of σ and σ /2 is 1.1σ implying a 10% error which we declare acceptable

THE ZEISS MIRROR MECHANISM

- Reimer 19[illegible]
- Pimpale 1[illegible]



- This mechanism, patented by BESSY and Zeiss, is a major reason for the success of this design
- The idea is to find a point about which to rotate the mirror such that the central ray always hits the grating pole - this can be done with only a few microns error
- The easy and less accurate solution is continue the mirror surfaces at maximum and minimum angle to intersect the *y* axis and take the average of the two points - this will be near *A* (0, *D*/2) for small angles
- More accurate solutions (Pimpale 1991) are close to *B* (0, 3*D*/2) - best solutions are good within 10µm if $D \leq 8$ cm and the grazing angle is less than 10° - *B* itself is a good solution to within 10 µm if $D \leq 3$ cm and the grazing angle is less than 10°

SOME WORKING CURVES FOR PGM'S

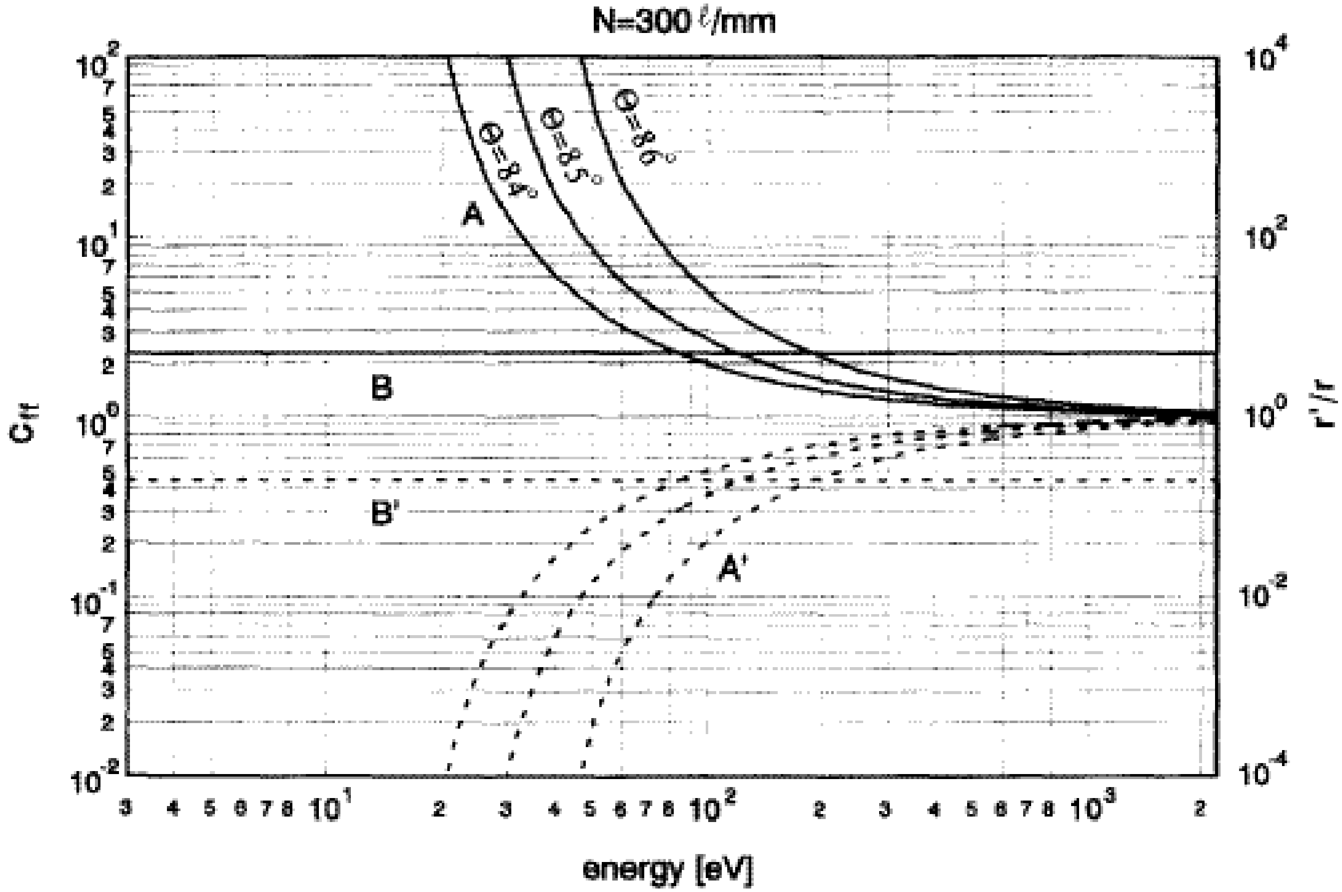
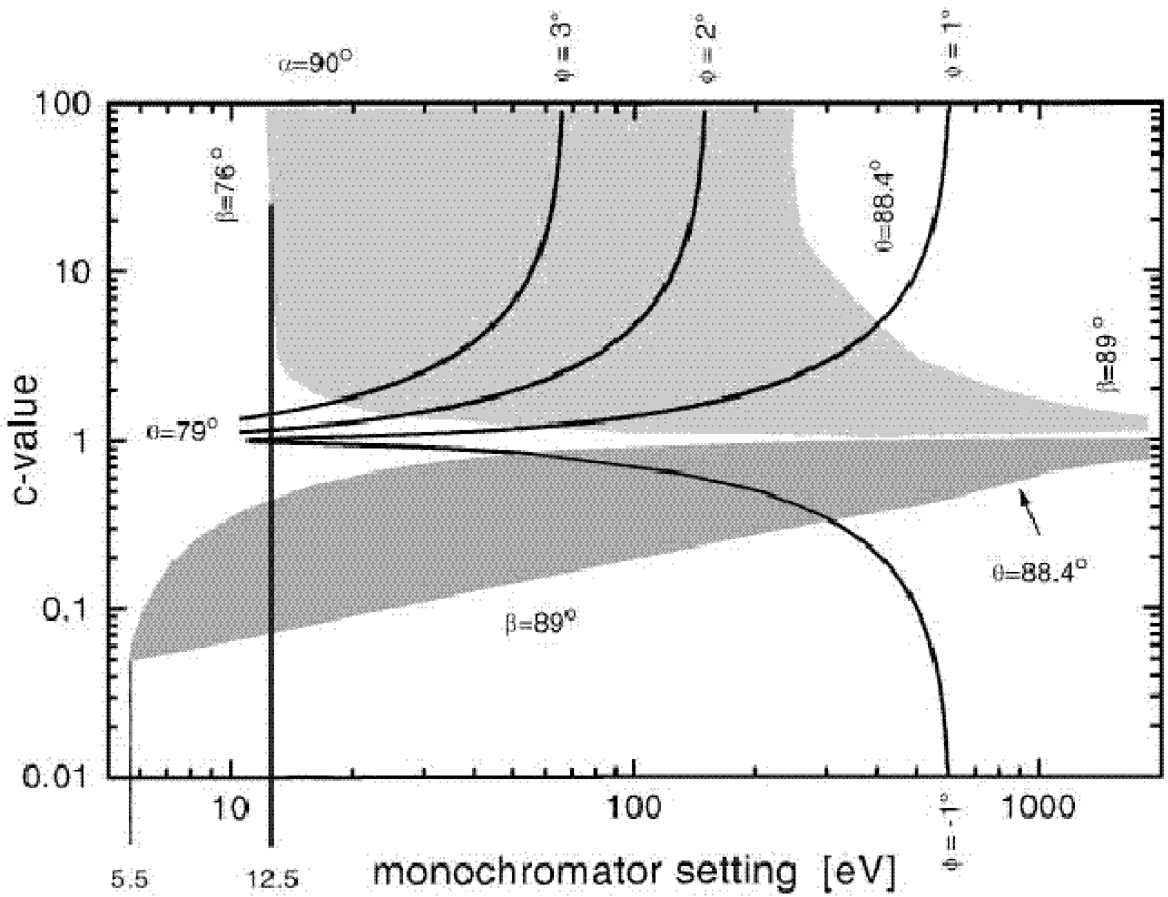


Fig. 1. Working curves for plane-grating monochromators with 300 lines/mm: (A) grating rotation at constant deviation $|\alpha| + |\beta| = 2\Theta$ = constant in inside diffraction order; (A′) the same but outside diffraction order; (B) fix-focus mode, $c_{ff} = 2.25$; (B′) fix-focus mode, $c_{ff} = 1/2.25$.

ACCESSIBLE RANGES OF THE SCAN PARAMETERS



- 300/mm grating
- 79°< θ <88.4°
- -89°< β <-76°

CONTRIBUTIONS TO THE SX700 RESOLUTION

Follath 1997, 2001

$$\frac{m\lambda}{d} = \sin\alpha + \sin\beta \quad \text{so} \quad \left(\frac{\partial\lambda}{\partial\alpha}\right)_{\beta} = \frac{d\cos\alpha}{m}$$

$$\frac{d\lambda}{dq} = \frac{d\lambda}{d\beta}\frac{d\beta}{dq} = \frac{d\cos\alpha}{mr'}$$

Fractional bandwidth due to the entrance slit is

$$\left(\frac{\Delta\lambda}{\lambda}\right)_{\text{source}} = \frac{\Delta q}{r} \; \frac{\cos\alpha}{m\lambda/d} \equiv \frac{s}{r} A(c_{\text{ff}})$$

Angular error

Normalized angular dispersion

In the small - angle approximation

$$A(c_{\text{ff}}) \quad \sqrt{\frac{d}{m\lambda} \; \frac{2}{\left(c_{\text{ff}}^2 - 1\right)}}$$

NB - the grating changes the angular spread by $1/c_{\text{ff}}$ (c_{ff} is the magnification)

$$\left(\frac{\Delta\lambda}{\lambda}\right)_{\text{source}} = \frac{s}{r} A(c_{\text{ff}})$$

$$\left(\frac{\Delta\lambda}{\lambda}\right)_{\text{exit slit}} = \frac{s'}{r'} c_{\text{ff}} A(c_{\text{ff}})$$

$$\left(\frac{\Delta\lambda}{\lambda}\right)_{\text{aberr}} = \frac{\Delta y'}{r'} c_{\text{ff}} A(c_{\text{ff}})$$

$$\left(\frac{\Delta\lambda}{\lambda}\right)_{\text{preopt}} = \sigma_{\text{po}} A(c_{\text{ff}})$$

$$\left(\frac{\Delta\lambda}{\lambda}\right)_{\text{focopt}} = \sigma_{\text{fo}} c_{\text{ff}} A(c_{\text{ff}})$$

$$\left(\frac{\Delta\lambda}{\lambda}\right)_{\text{grating}} = \sigma_{\text{gr}} \left(1 + c_{\text{ff}}\right) A(c_{\text{ff}})$$

$$\left(\frac{\Delta\lambda}{\lambda}\right)_{\text{total}} = \sqrt{\sum_i \left(\frac{\Delta\lambda}{\lambda}\right)_i^2} = \frac{1}{R}$$

RESOLUTION CONTRIBUTIONS FOR A BESSY PGM

Follath 2001

BESSY U125/1-PGM

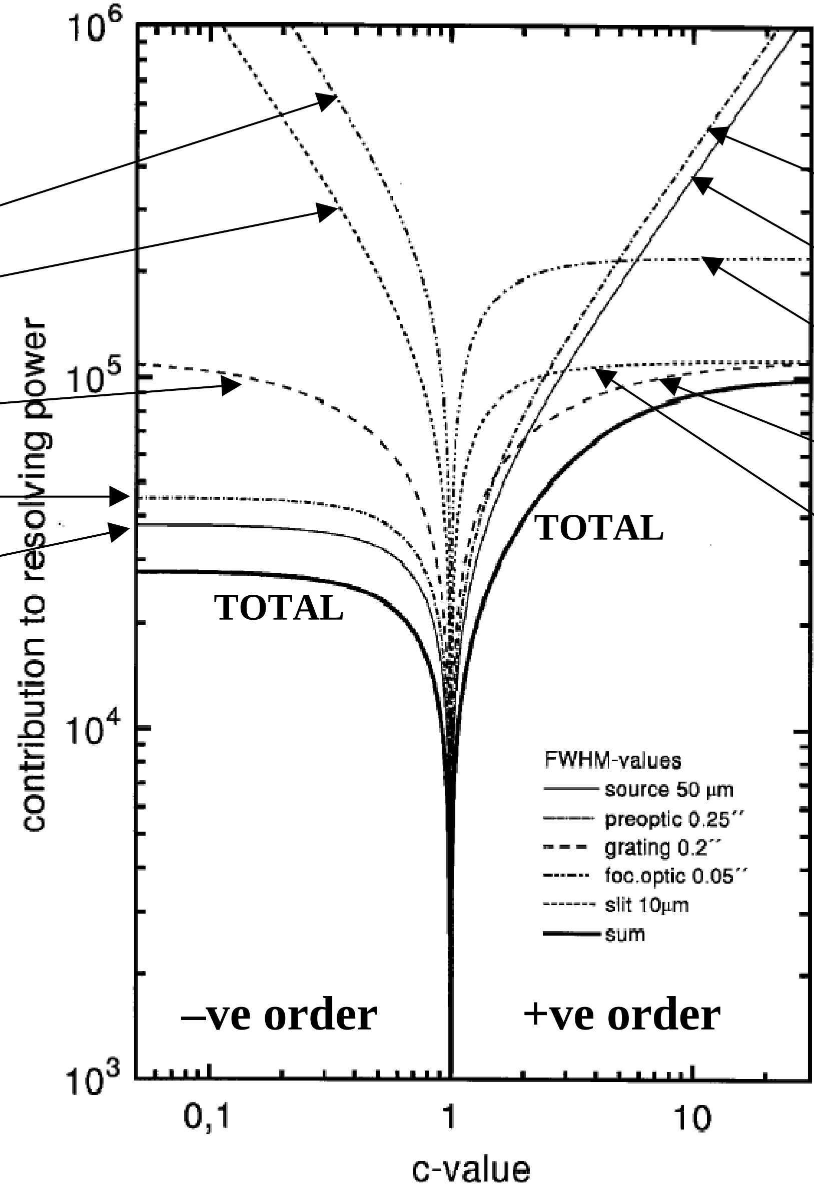
Foc optic 0.05 sec

Slit 10 µm

Grating 0.2 sec

Preoptic 0.25 sec

Source 50 µm



BESSY U125/1-PGM

Preoptic 0.25 sec

Source 50 µm

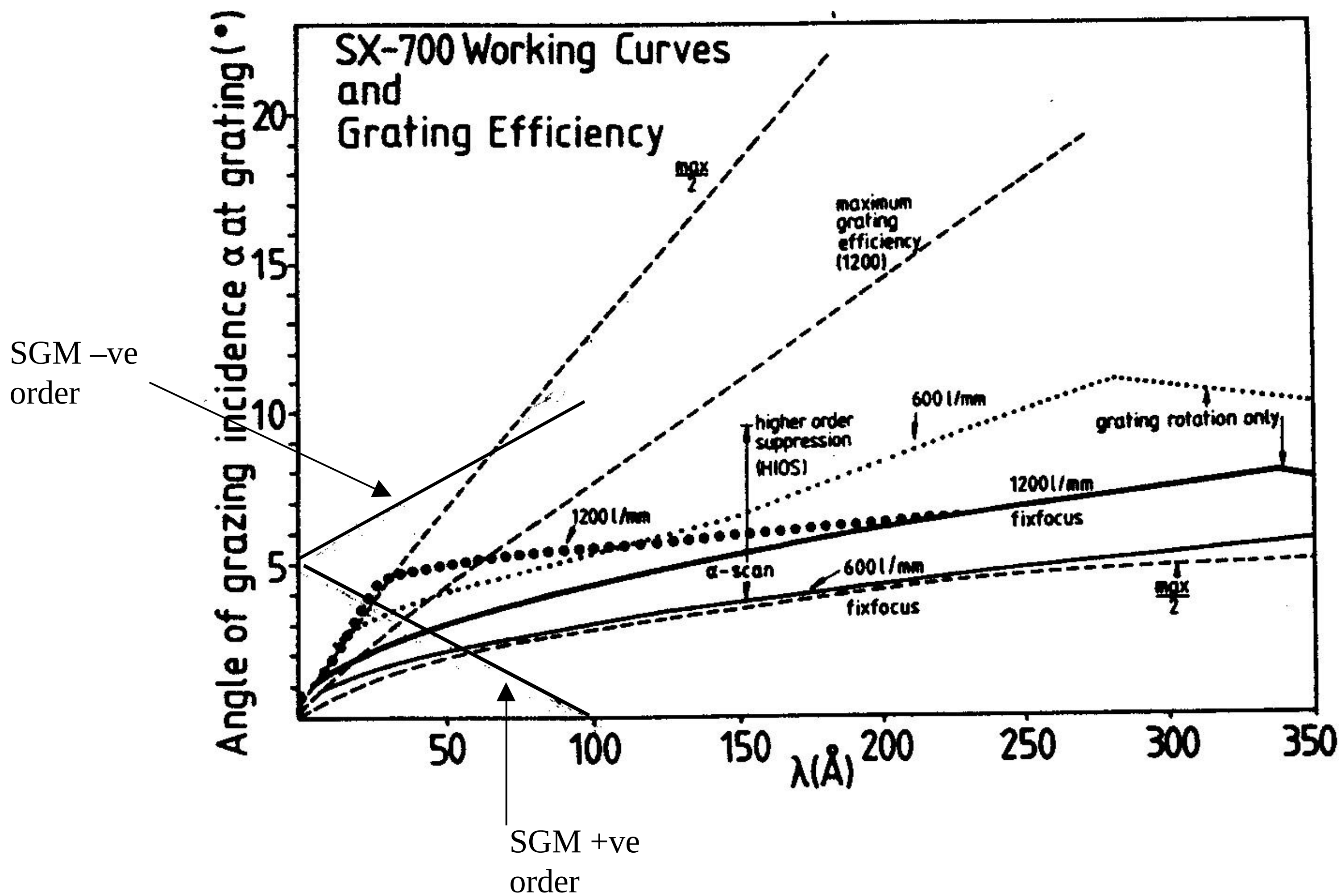
Foc optic 0.05 sec

Grating 0.2 sec

Slit 10 µm

WORKING CURVES FOR c_{ff}=2.25 ETC

Petersen 1986



BESSY CLSX700'S: SUMMARY

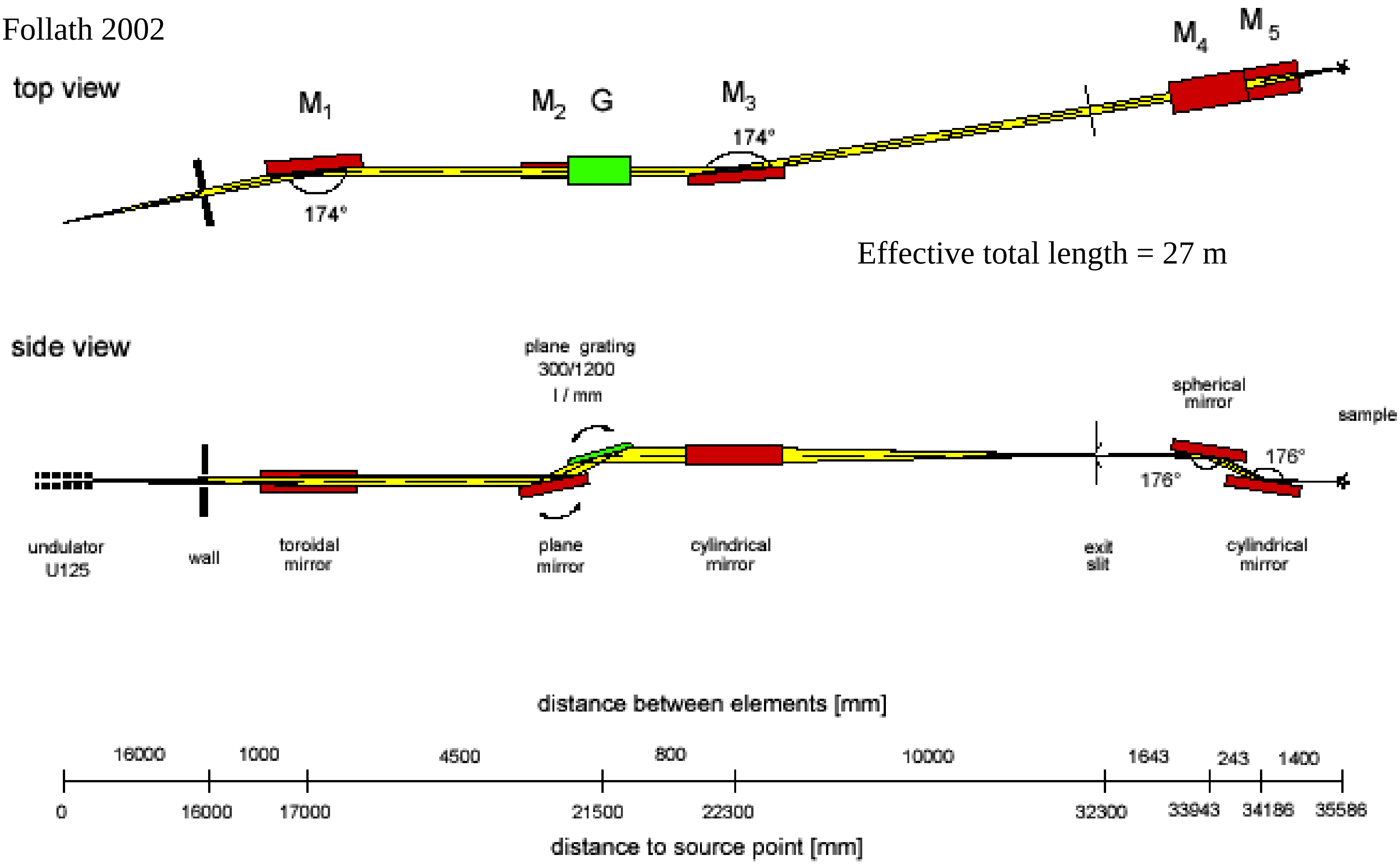
Table 1
Operational collimated plane grating monochromators at BESSY II

Beamline	Energy range (eV)	Resolving power	Dedication
U125/1-PGM	15–600	100.000[a]	low energy beamline
UE56/1-PGM	60–1500	100.000[a]	circularly polarised, two chopped beams
UE56/2-PGM1	"	110.000[a]	"
UE56/2-PGM2	"	110.000[a]	"
U41-PGM	170–2000	6.000[b]	high energy, high flux, small focus
U49/1-PGM	130–2000	10.000[b]	PEEM
U49/2-PGM2	80–2000	10.000[b]	PEEM
U180-PGM	30–1900[c]	30.000[a]	reflectometry, high spectral purity

[a] Aligned and determined with helium $(2-1_3)$-profile.
[b] Aligned and determined with $N_2: 1s \rightarrow \pi^*$ core hole absorption.
[c] Wiggler mode of the insertion device.

BESSY U125/1-PGM BEAM LINE

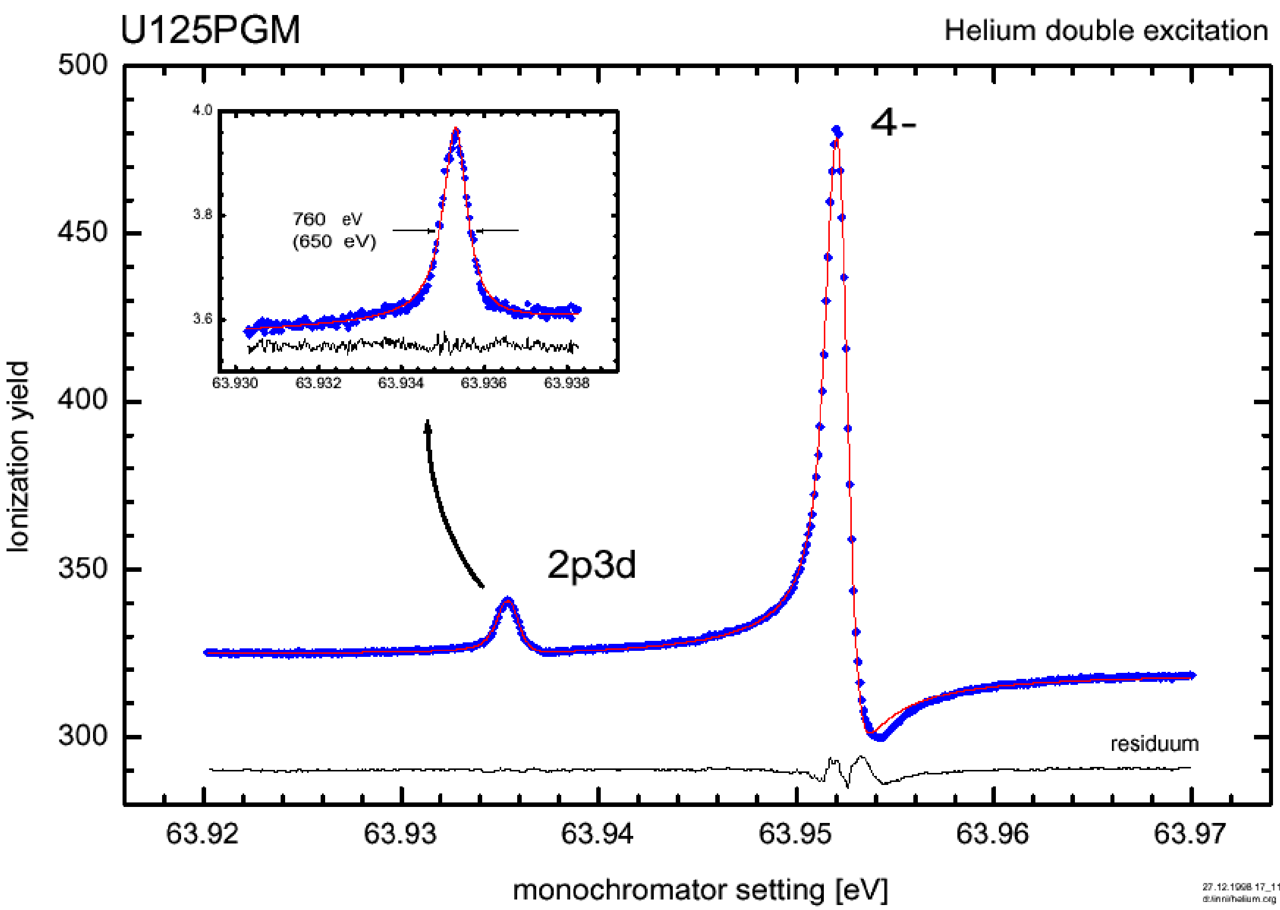
Follath 2002



Effective total length = 27 m

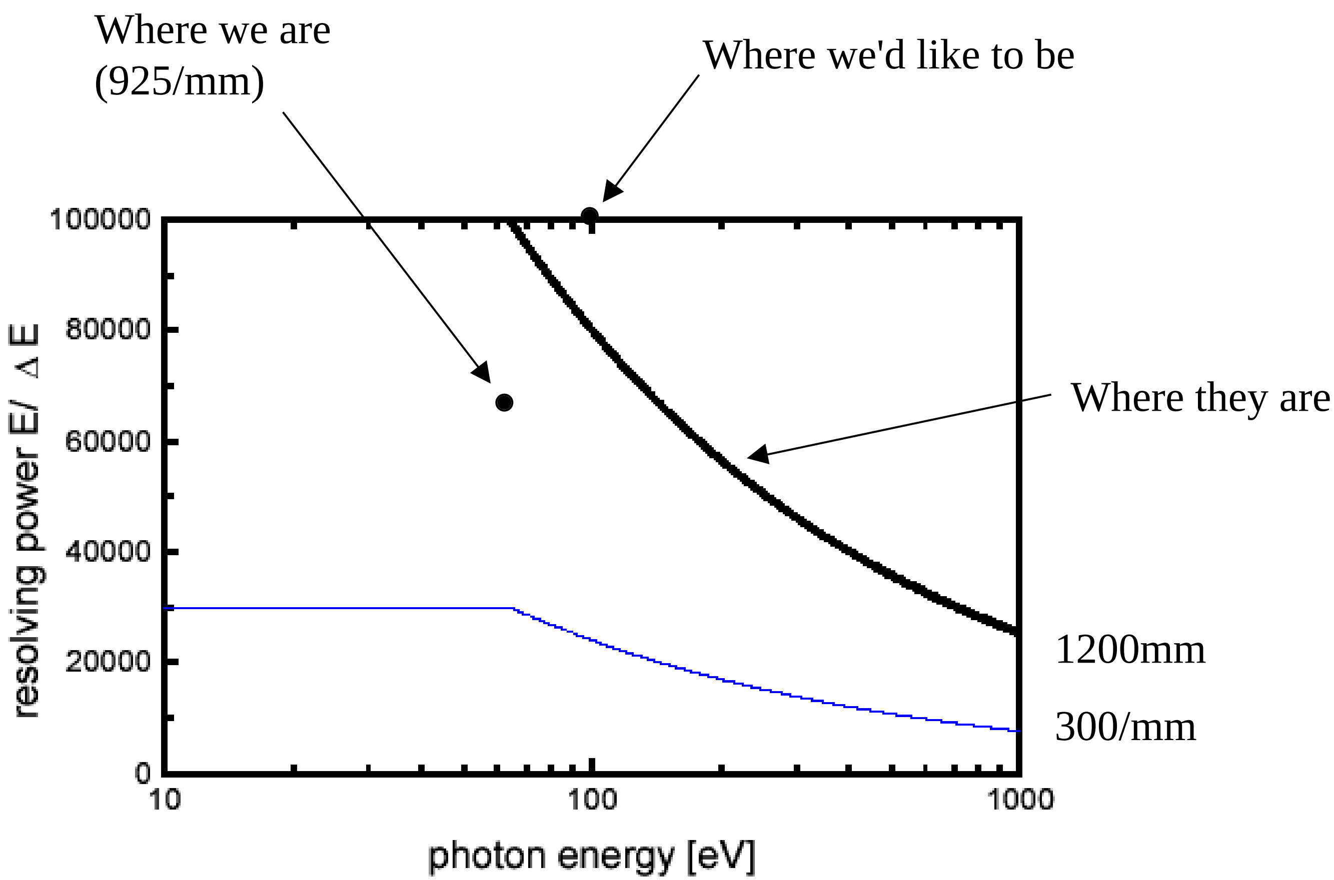
BESSY PGM RESOLUTION DEMONSTRATION

Picture from R. Follath, BESSY



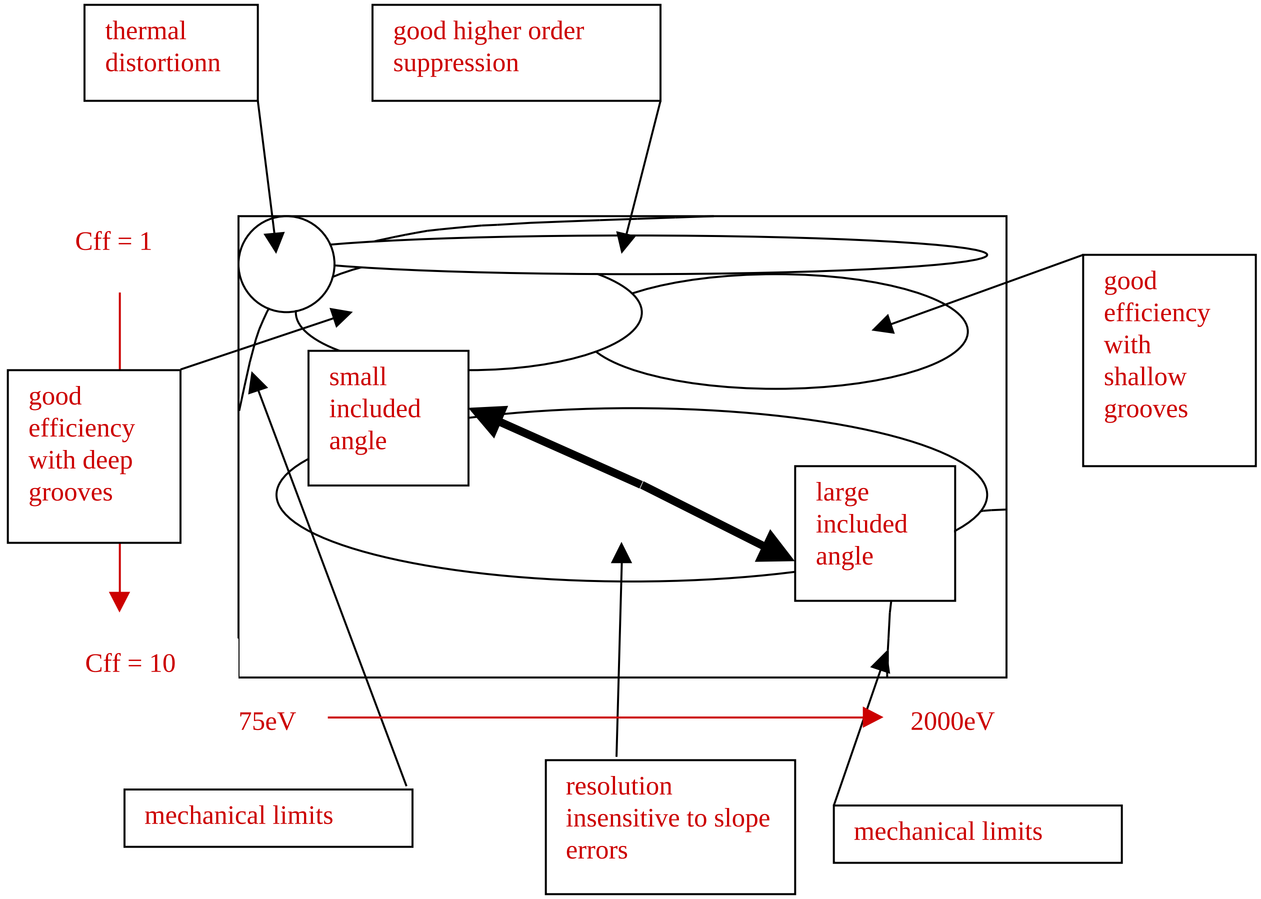
- Doppler width 0.4 meV
- Monochromator contribution 0.65 meV
- Resolving power=1.0x10^5
- Rotation increments
  - grating: 17 nrad
  - mirror: 9 nrad
- Measured with 1200/mm grating at c_{ff} =10 to 12

BESSY PGM'S: RESOLUTION SUMMARY



Slide from Tony Warwick

Mono angles



Parameters for this study:

150 lines/mm (low dispersion)	25nm groove depth	(operating from 75 eV to 800eV)
1200 lines/mm (high dispersion)	6nm groove depth	(operating from 300 eV to 2000eV)

OPTICAL PATH FUNCTION: VARIED-LINE-SPACING GRATINGS

Now the groove spacing $d(w)$ and number n(w) are functions of w and are also expressed as power series

$$d(w) = d_0\left(1 + v_1 w + v_2 w^2 + \ldots\right) \qquad n(w) = \sum_{i=1}^{\infty} n_{i00} w^i$$

So the optical path function becomes

$$F = \sum_{ijk} C_{ijk}(\alpha, r) w^i l^j z^k + \sum_{ijk} C_{ijk}(\beta, r') w^i l^j z'^k + \frac{m\lambda}{d_0} n_{ijk}$$

$$n_{100} = 1$$

$$n_{200} = -v_1/2$$

$$n_{300} = \left(v_1^2 - v_2\right)/3$$

$$n_{400} = \left(-v_1^3 + 2v_1 v_2 - v_3\right)/4$$

$$n_{ijk} = 0 \quad \text{if } i \text{ or } k \neq 0$$

Evidently the use of VLS can benefit aberrations of the form $i00$:

Defocus, coma, spherical aberration but not ones with $j, k \neq 0$

WHY DO VLS GRATINGS WORK?

The spherical - grating focus condition is now:

$$(F)_{200} = \frac{1}{2} w^2 \left\{ \left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} \right) + \left(\frac{\cos^2 \beta}{r'} - \frac{\cos \beta}{R} \right) - \frac{v_1 m \lambda}{d_0} \right\} = 0$$

So setting $R = \infty$, using the grating equation and switching to grazing angles a, b

$$\frac{1}{r'} = \frac{\cos a - \cos b}{\sin^2 b} - \frac{1}{r} \frac{\sin^2 a}{\sin^2 b} = \frac{1}{r} \left\{ v_1 r \frac{-2 \sin\left(\frac{a+b}{2} \right) \sin\left(\frac{a-b}{2} \right)}{\sin^2 b} - \frac{\sin^2 a}{\sin^2 b} \right\}$$

Now approximating $\sin a$ a etc

$$\frac{1}{r'} = \frac{1}{r} \left\{ -v_1 r \frac{a^2 - b^2}{2b^2} - \frac{a^2}{b^2} \right\}$$

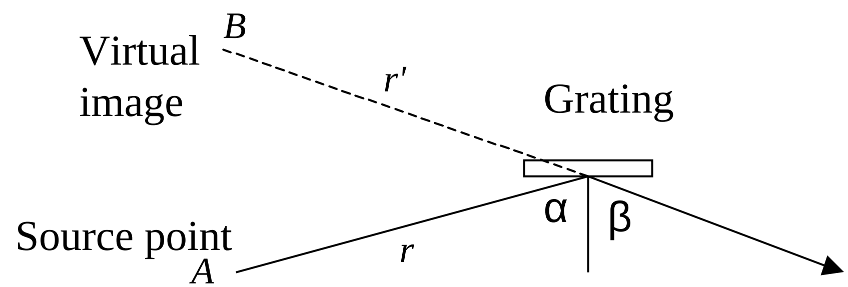
Evidently if $v_1 = \frac{-2}{r}$ then $r' = -r$

IDENTICALLY (for all values of a, b

and thus λ. Moreover if, in addition,

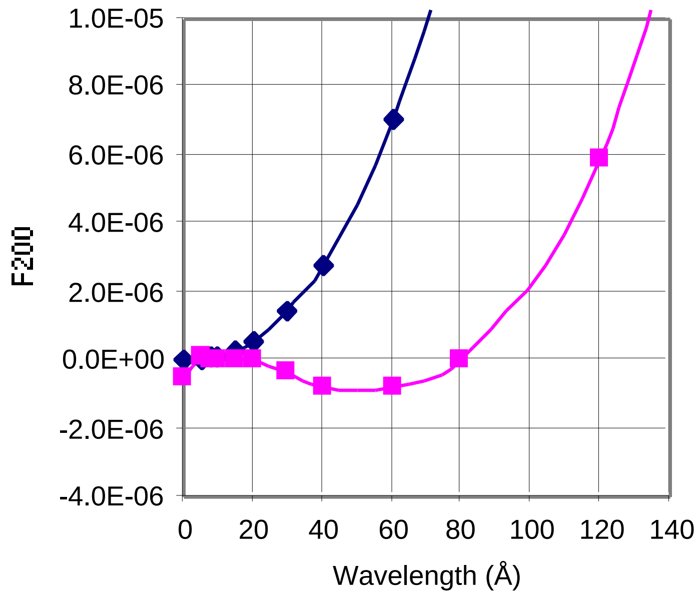
$v_2 = \frac{1}{r^2}$ then coma and sperical aberration

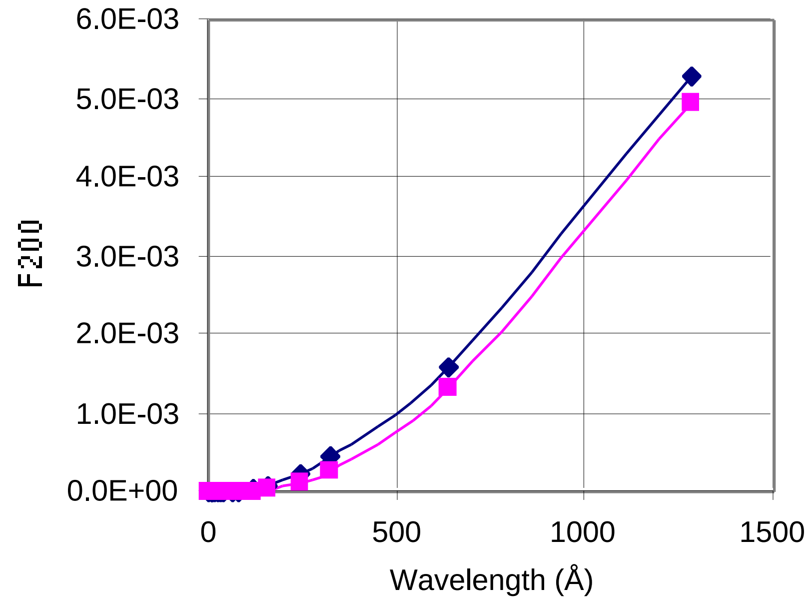
are corrected as well under the same small - angle assumption



This works equally well in converging or diverging light (principle of reversibility) although the literature discusses only converging.

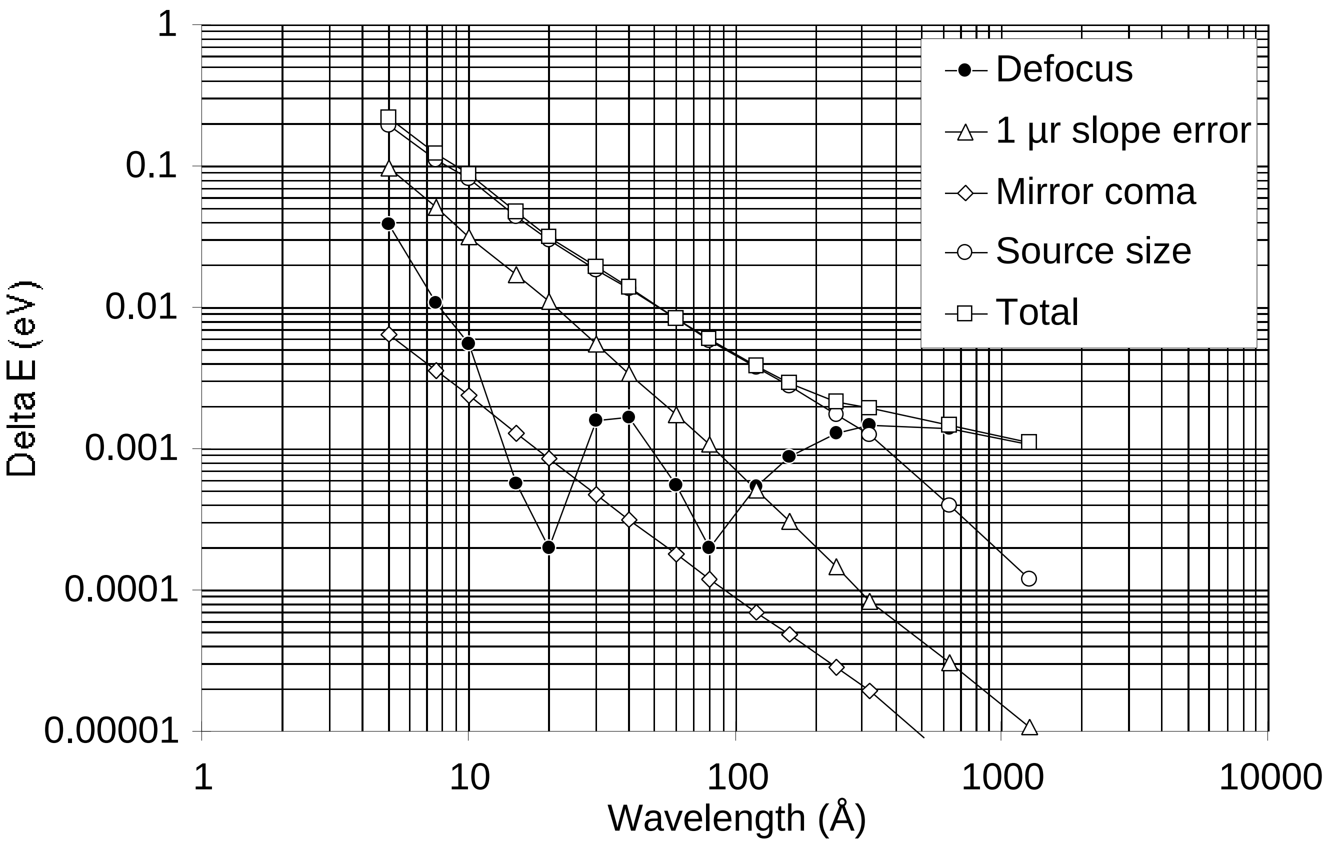
DOES $v_1 = -r/2$, $r' = -r$ GIVE OPTIMUM FOCUSING?





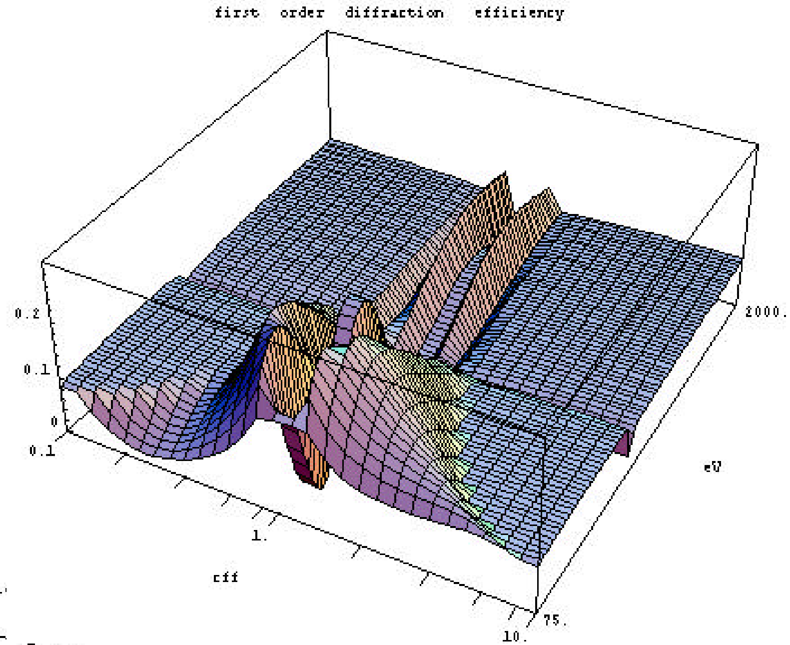
- No - the usual procedure is to write the focus equation twice for two wavelengths of exact focus and solve for r' and v_1 - (this requires a fixed included angle or at least a fixed focusing principle) - the nominal focal distance then changes by a small amount (2% in the above case) - this gives locally better focus although not much improvement over a large range
- Note that all of the design studies in the literature except one (Koike 1995) consider only *fixed-included-angle* cases and offer, sometimes very good, although still approximate solutions but they have SGM-like disadvantages.
- Now that the variable-included angle schemes are available we have *exact* focus solutions such as CLSX700 or classical SX700 although the latter does not give control of the included angle to the user.
- Therefore retrofitting VLS to a standard SX700 makes some sense to give user control of the included angle however note that the focal length or the focal distance of the mirror would have to change.
- Conclusion: VLS role in general-purpose monochromators is becoming minor but it is still strong in spectrographs.

VLS RETROFIT TO AN SX700

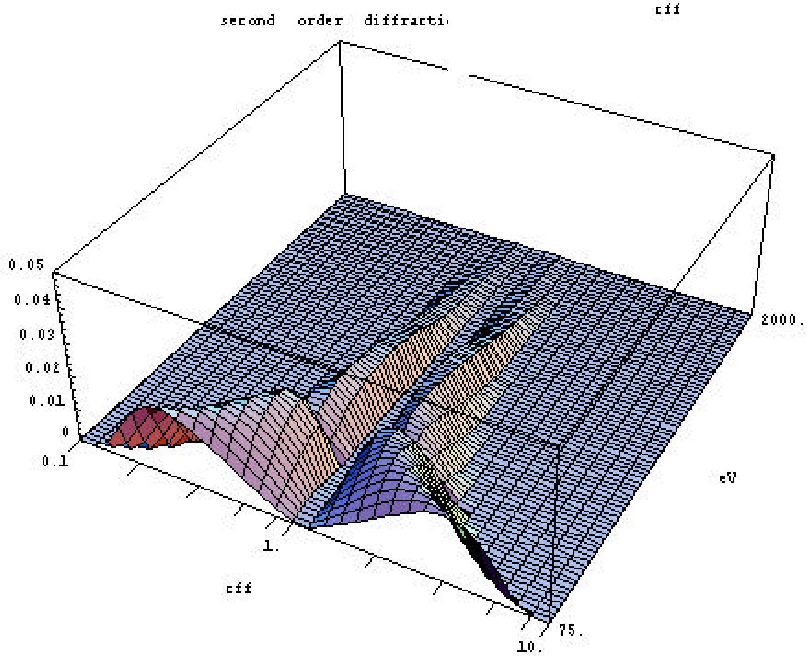


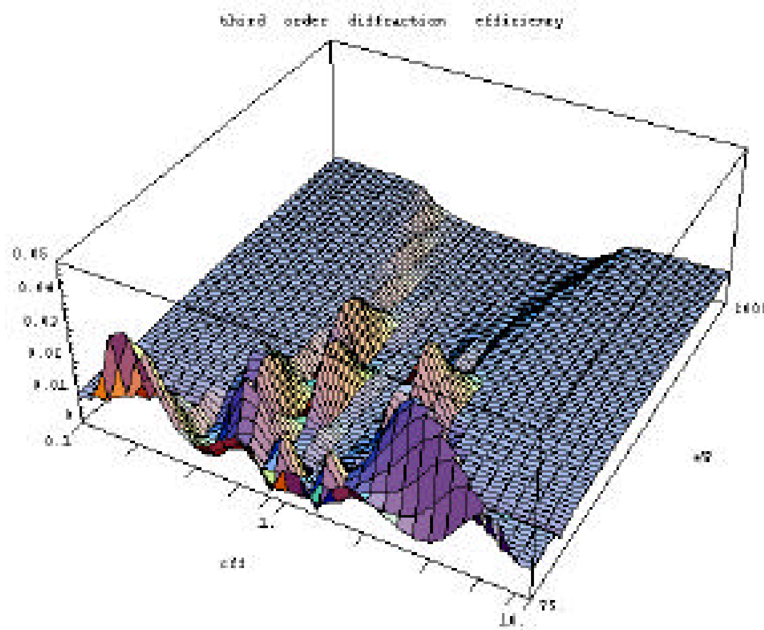
- VLS solution with c_{ff} chosen for maximum efficiency (between 1.5 and 2.5)
- Wavelengths of exact focus: 20 Å and 80 Å
- Source: size 50 μm and distance 15 m
- Beam height: 2mm
- Inside (+ve) order
- 1200/mm

MES PROJECT CALCULATIONS



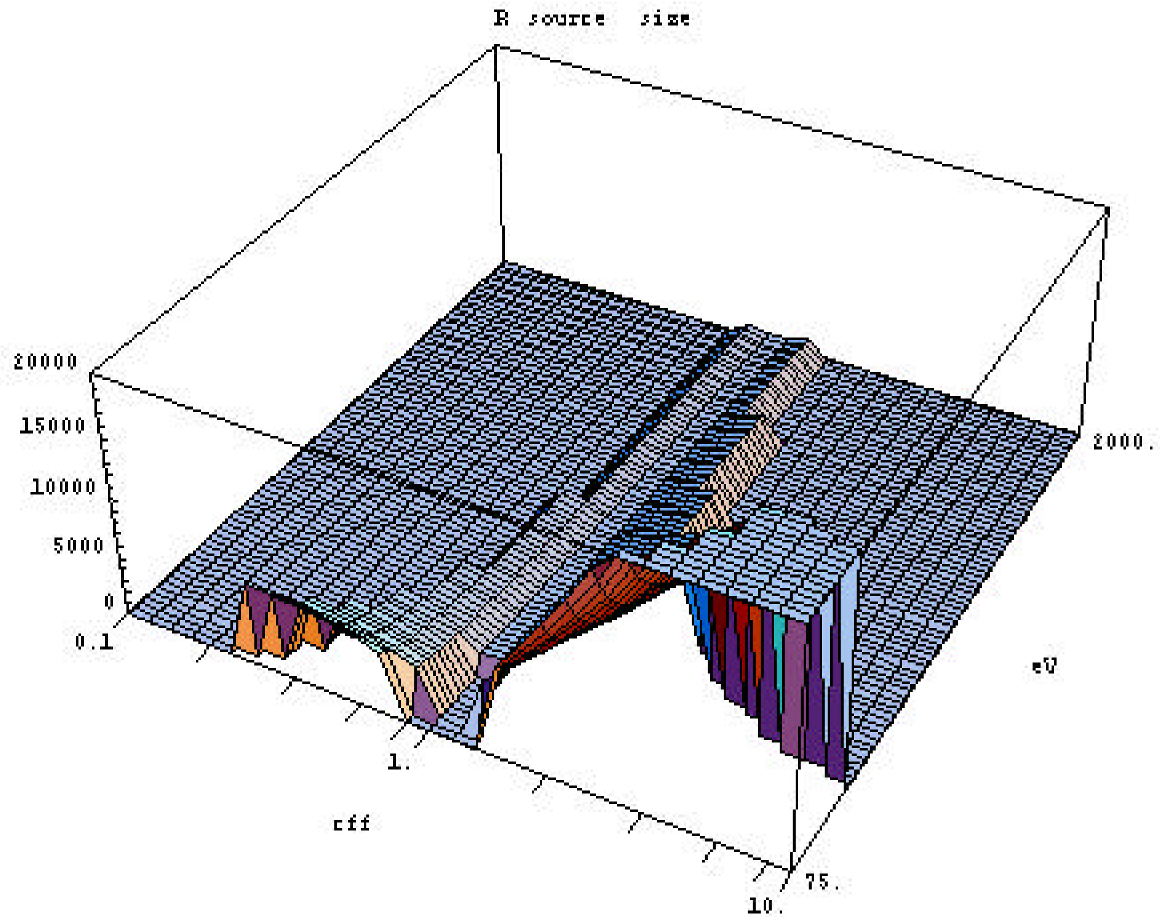
First, second and third order efficiency calculations for a laminar grating 150/mm





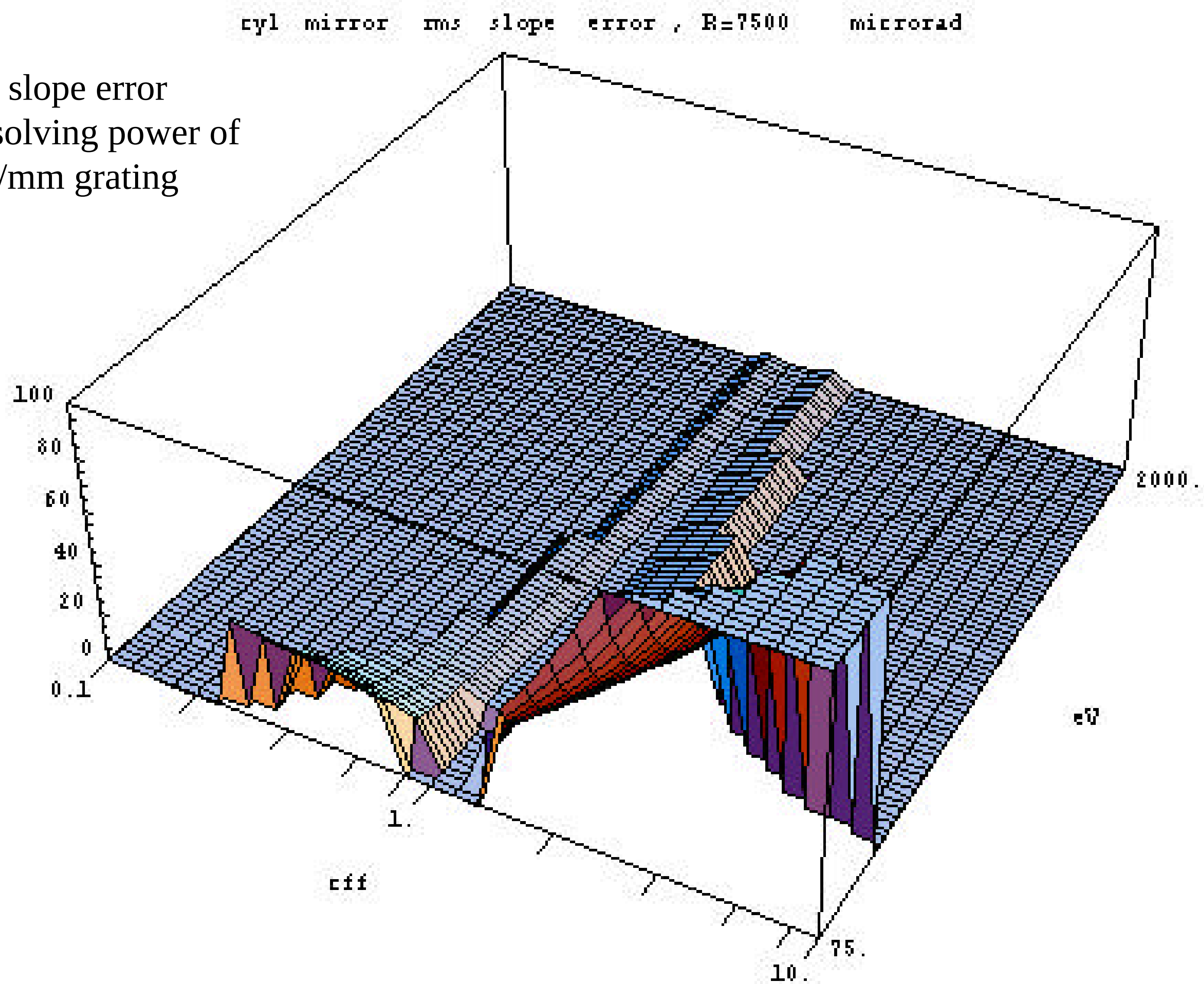
MES PROJECT CALCULATIONS

Source-size-limited resolving power for
a source of size FWHM = 40 μm at
distance 12 m with a 150/mm grating



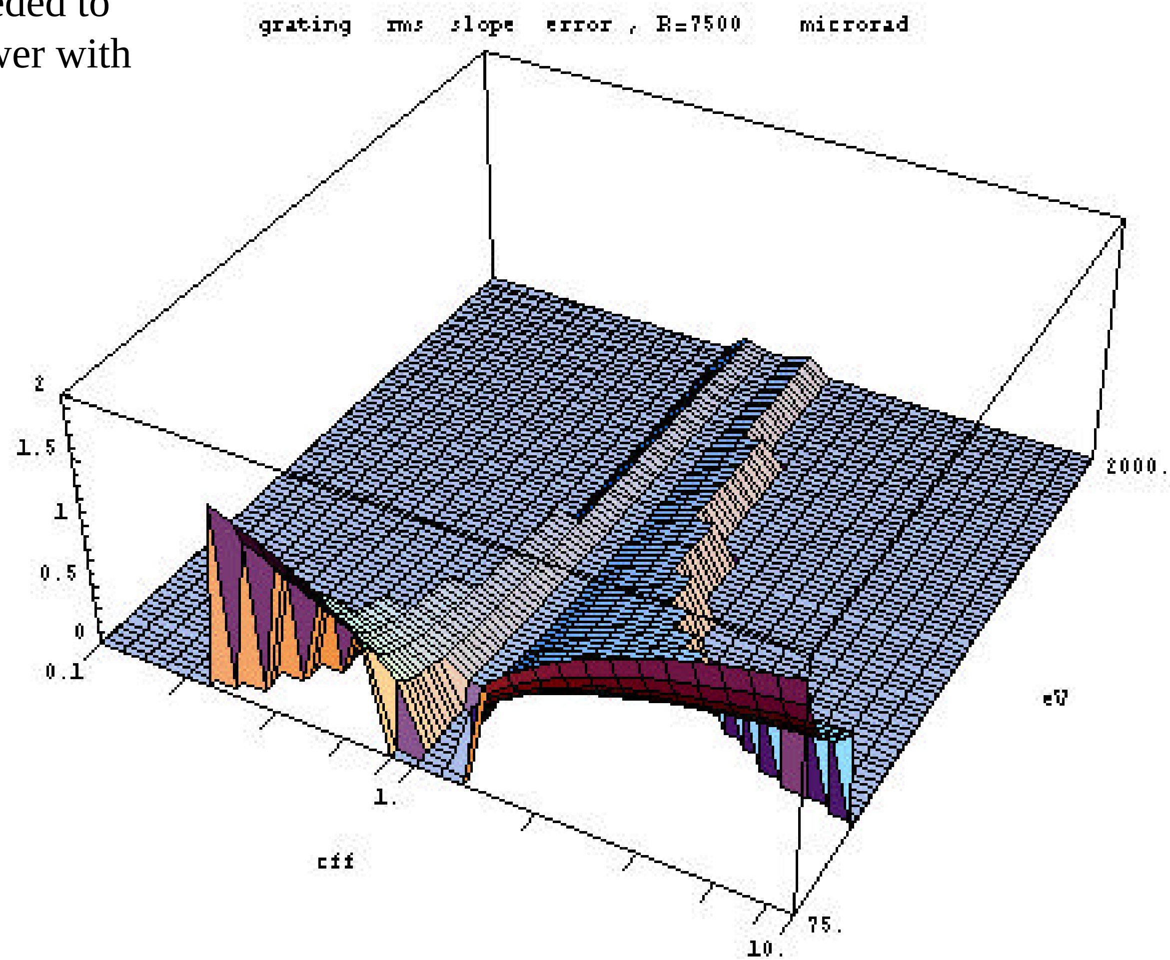
MES PROJECT CALCULATIONS

Cylindrical mirror slope error needed to get a resolving power of 7500 with the 150/mm grating

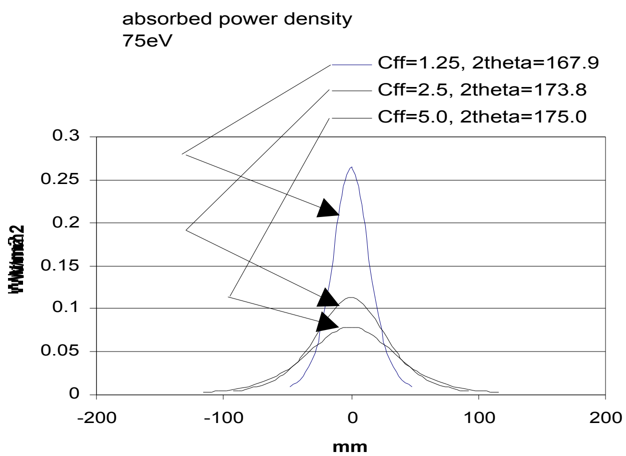


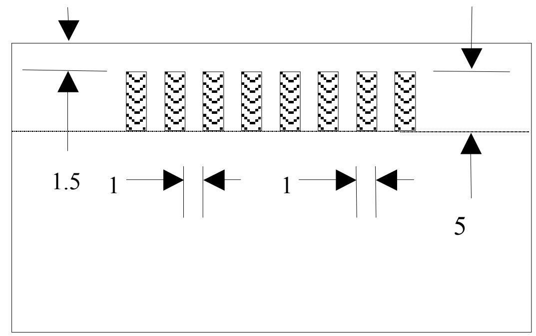
MES PROJECT CALCULATIONS

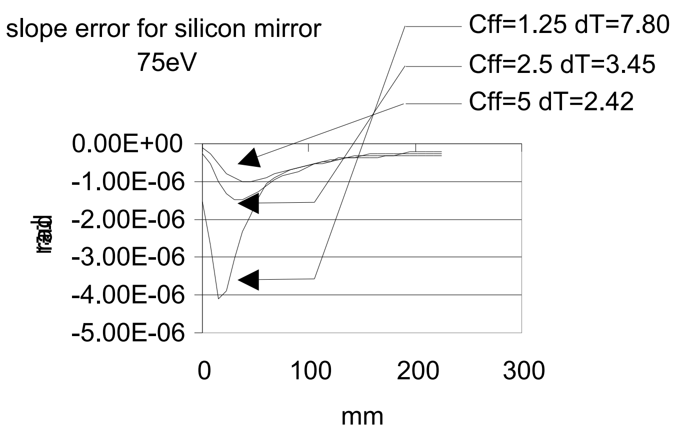
Grating slope error needed to get 7500 resolving power with 150/mm grating



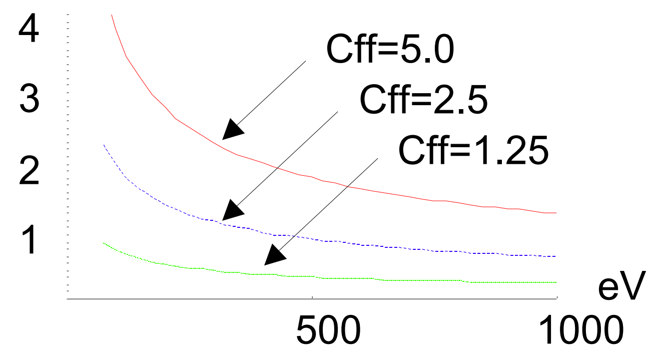
Mirror cooling for high heat load at low energy (75eV)







The rms slope error (μrad) of the pre-mirror corresponding to a resolving power R=7500 (FWHM) from the 150l/mm grating.



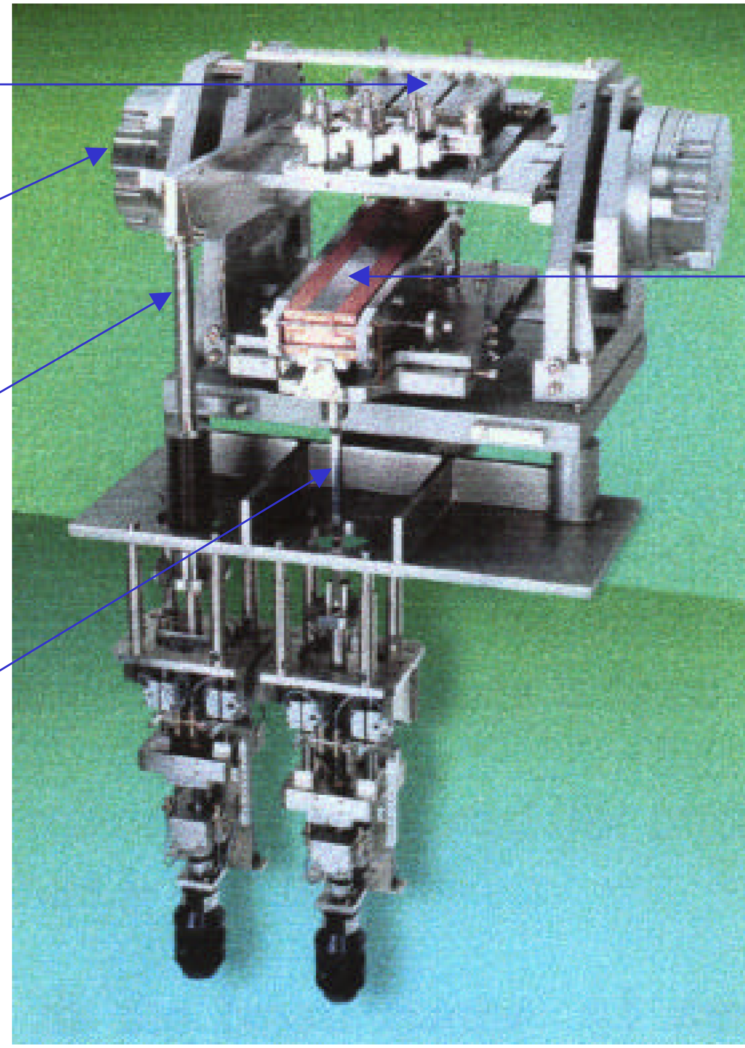
JENOPTIC SX700 MONOCHROMATOR

Three gratings

UHV rotary encoder

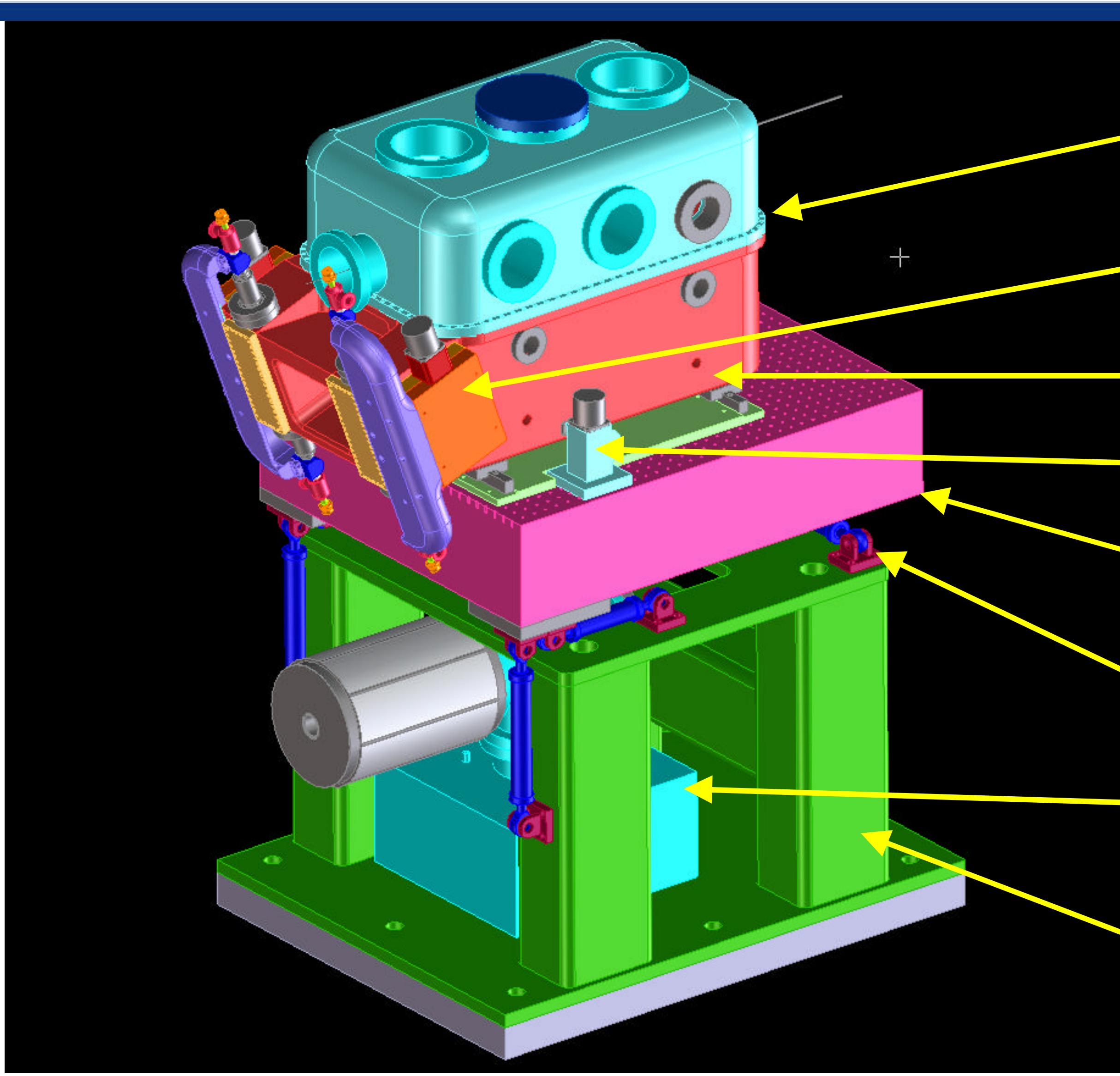
Grating drive arm

Mirror drive arm



Plane mirror

New implementation of SX700 monochromator



Seal joint below beam height for alignment access

External sine-bar drives and linear encoders

Aluminum structural vessel

External grating changer

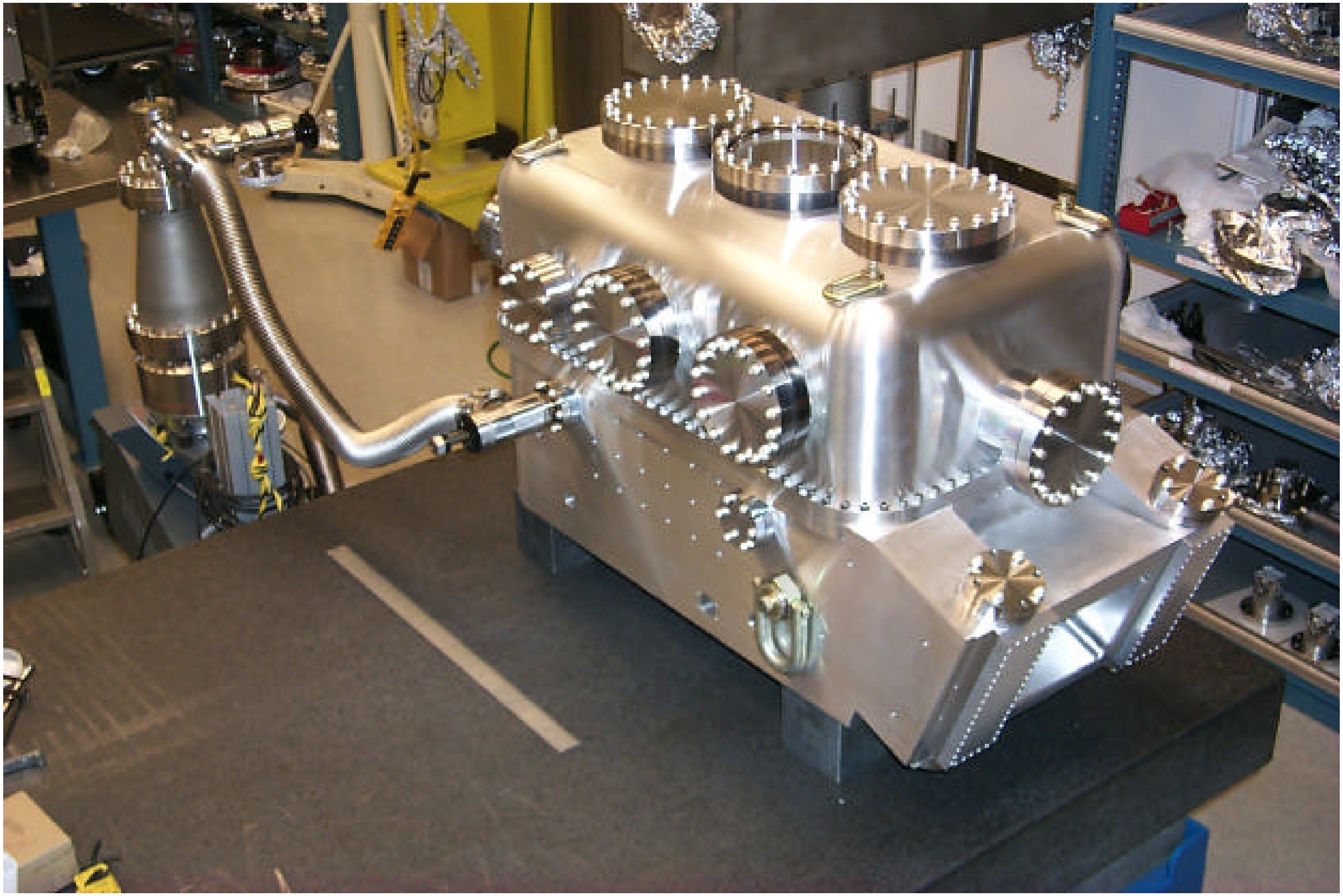
Lightweight rigid honeycomb table

6-strut alignment

Heavy pump below bellows on separate support

Legs filled with epoxy granite

Monochromator chamber, vacuum test Oct 2001



monochromator scanning mechanism with integral cooling